Agent Design and Performance

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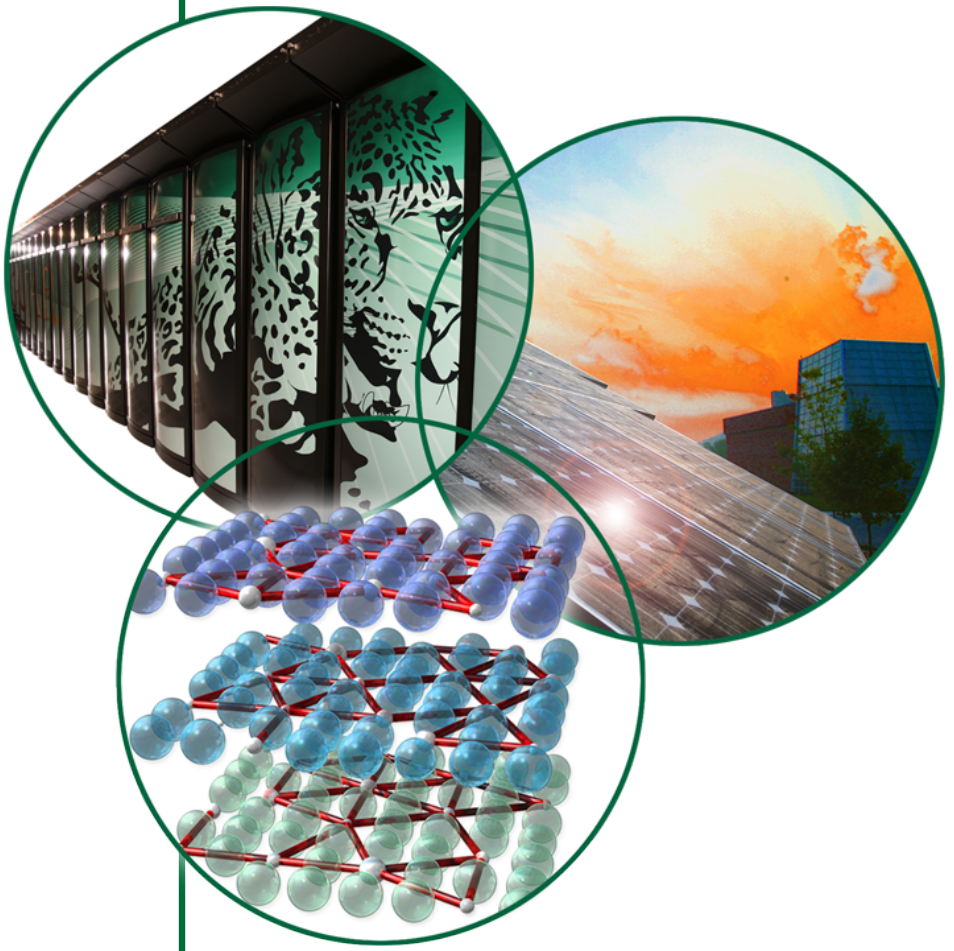


NEAMS PI Meeting

L'Enfant Plaza Hotel, Washington DC

18-20 October 2010

U.S. DEPARTMENT OF ENERGY

Safeguards & Separations

OAK RIDGE NATIONAL LABORATORY

MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

SafeSeps IPSC Challenge Problem:

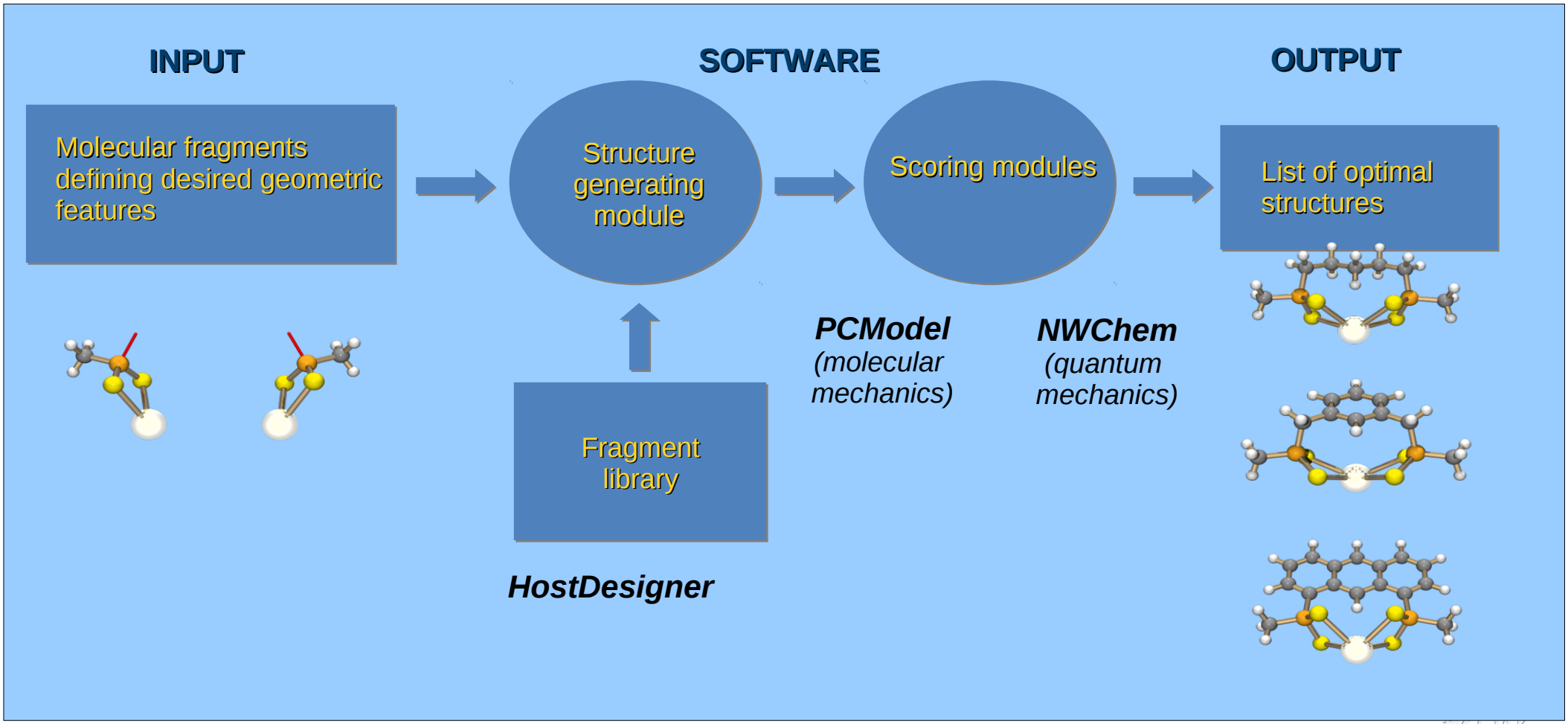
Agent Design to Process Design

- **Description:** Develop molecular design software to predict performance of sequestering agents for applications in separation of specific radionuclides from nuclear fuel reprocessing plant streams:
  - Improved selectivity, binding affinity, and aqueous insolubility
  - Improved ion-exchange
  - Improved interfacial transport behavior

- **Impact:** *NE R&D Objective Three*. Highly selective separating agents will be needed to meet the needs associated with future fuel cycles and responsibly disposing of nuclear waste:
  - Save significant cost in agent identification, evaluation and deployment.
  - Key need of Separations and Waste Forms Technical Area of the Fuel Cycle R&D Program (Minor Actinide Sigma Team).

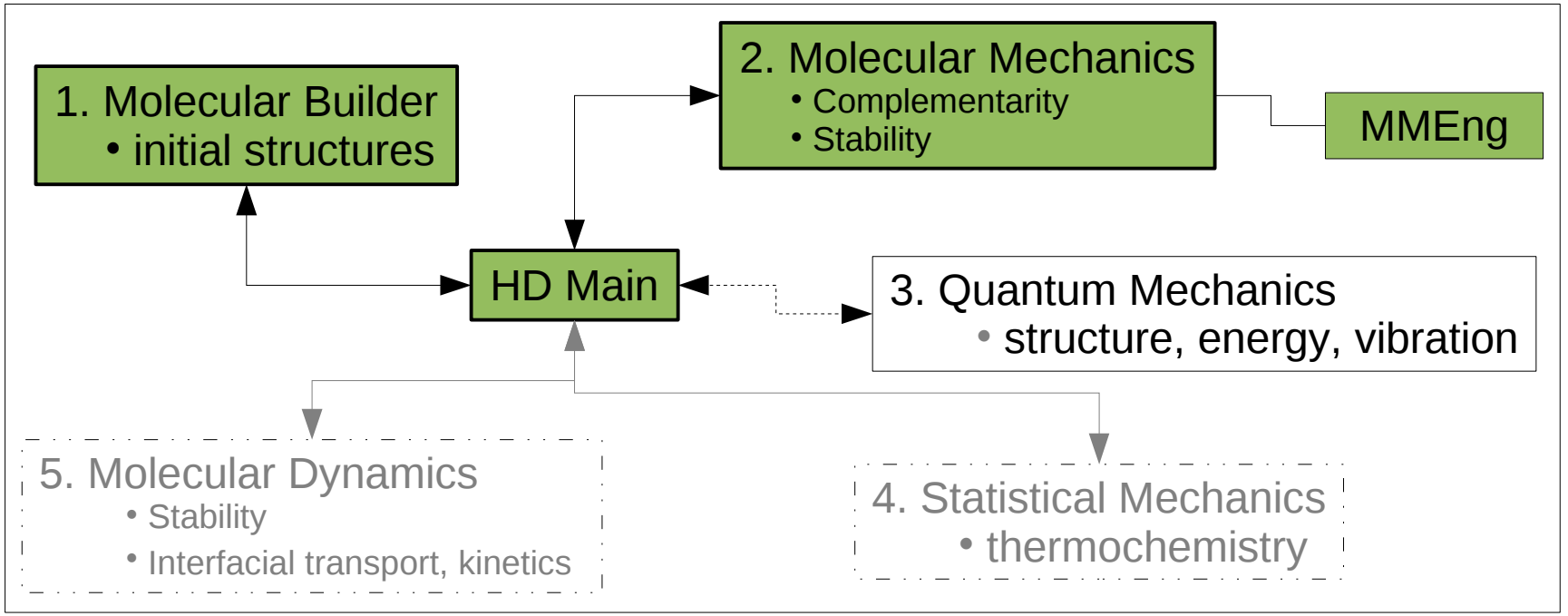
New ligands for selective complexation of metal ions (HostDesigner)

Computer-aided, structure-based design of radionuclide sequestering agents is being used to guide experimental programs. Increase in fragment library size and need for more accurate scoring motivates adapting this system for supercomputers.



Activity:

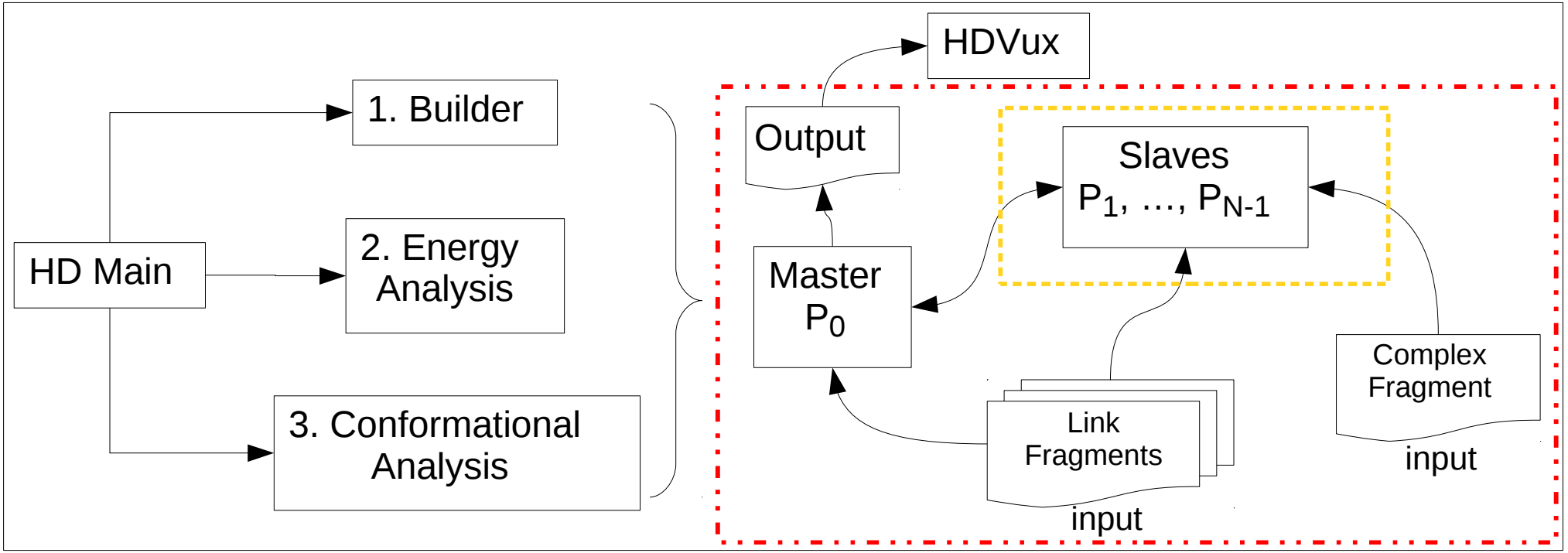
Develop molecular-level codes for ligand design and performance analysis



- **FY10 Tasks**
  - ✔ Modifications of HostDesigner code
    - ✔ Reorganization to allow for coupling of new modules
    - ✔ Parallelization of molecular mechanics modules
  - ✔ Identification of coupling with quantum mechanics libraries
  - ✔ Testing

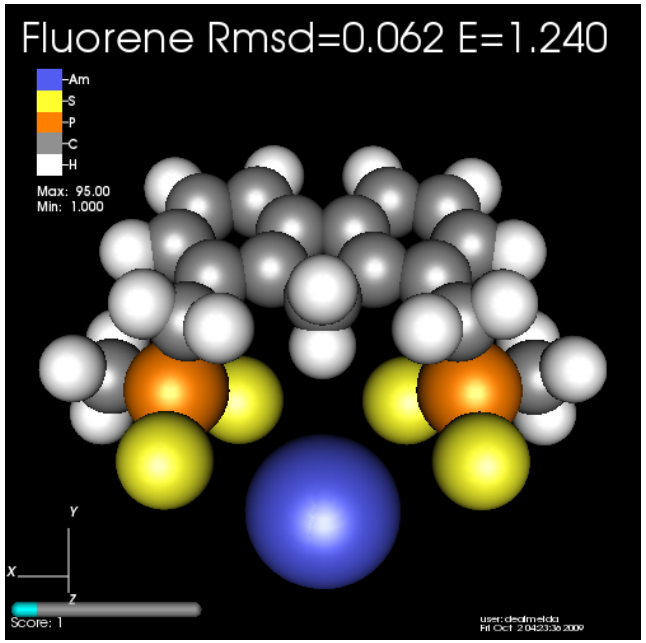
Progress on Parallelization

- Parallelization of Host-Designer active items
  - Master-slave approach for balancing the computational work
  - Planning parallel IO



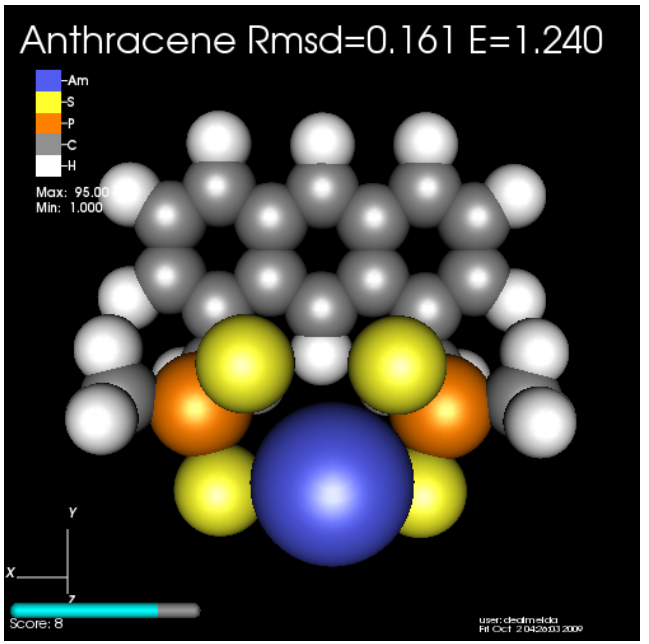
Verification against sequential code results

- Americium dimethylphosphinate chelate complex fragment



asymmetric

candidates



1st candidate

8th candidate

- Parallel results match sequential code
- Ligand suggested for synthesis by Minor Actinides Sigma Team

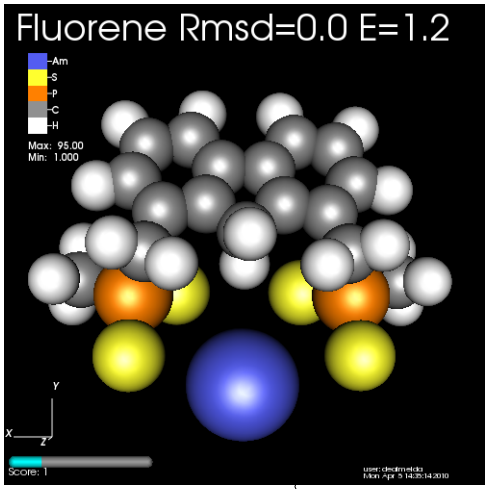
Testing:

Americium ligand (Minor Actinides Sigma Team)

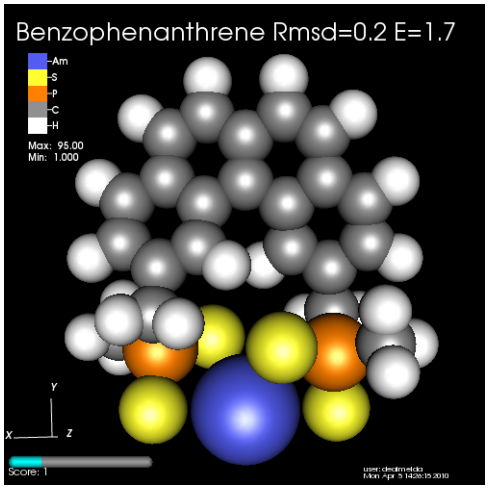
Library – 8 266 Links			
# Proc's	Build (2 188 candidates)	Complementarity (2 188 candidates)	Stability (1 024 candidates)
1024	2.5 min	2.7 min	98.8 min

- Previous simulation capability: limited MM analysis on 10 to 20 ligands (~days wall-clock time)
- Current capability: MM conformer search on > 1000 ligands in ~1.5 hours wall-clock time

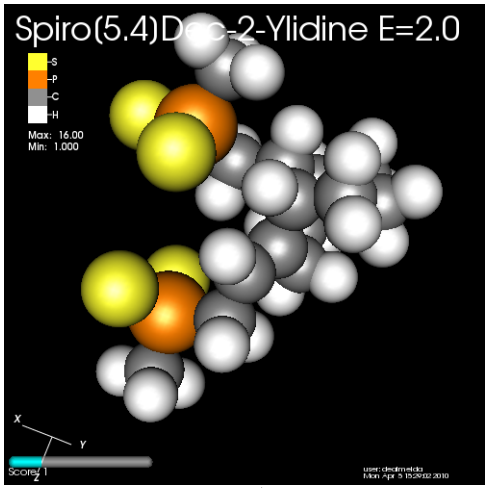
Build phase



Complementarity phase



Conformer phase



top candidates in each phase

- Modularized and integrated molecular mechanics module tested on Cray-XT5 parallel machine.
- New MPI version of the code to be used in FY10 Minor Actinides Sigma Team work.

Cluster Computing Testing

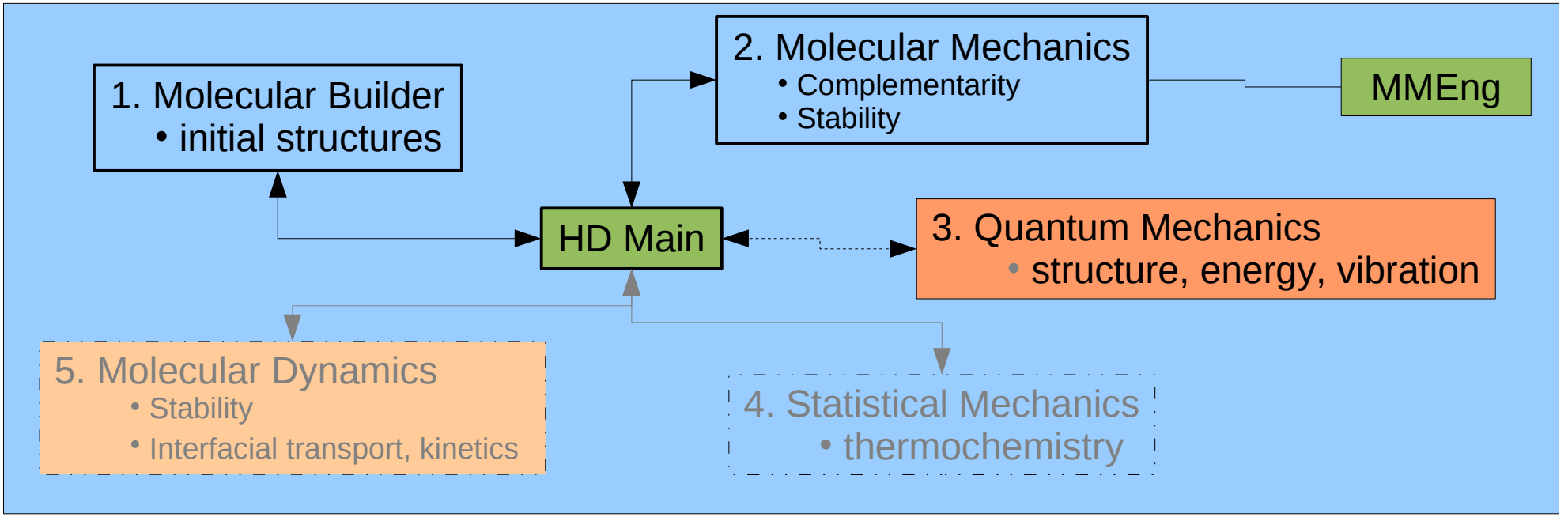
Library – 8 266 Links			
# Proc's	Build (1 094 candidates)	Complementarity (1 094 candidates)	Stability (256 candidates)
256	2.0 min	1.0 min	74.0 min

- INL CAMS cluster Helios
- Demonstrated portability on common linux cluster environment
- Potential source of CPU cycles for production runs by FCR&D users
- Would like access to more powerful machines for QM calculations

Outlook

Status, issues, and FY 11 work

- Sigma Team users now equipped with more powerful design capability needed in FY10
  - Experimental testing of synthesized molecules indicated promising extraction performance
  - But poor resistance to chemical environment
- Molecular mechanics module will require further development:
  - Potential rewrite of MMEng code or replacement by existing MM engine
- Module integration may benefit from software architecture analysis or use of a framework



- Quantum Mechanics module will be integrated next (NWChem parallel library)
  - Greatest impact of massively parallel computing to agent design and performance